FINAL REPORT OF RESEARCH PERFORMED UNDER
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This grant was awarded in 1965 and continued through 1970. It provided mainly for summer support of the two principal investigators, support for one or two graduate students, travel and computing funds. The following is a brief description of the research problems investigated during the period of the grant.

The first work concerned the calculation of photo-ionization cross sections near auto-ionizing lines (resonances). A method similar to the configuration interaction technique for improving bound state wave functions was developed for continuum states and applied to the ^1P resonances in the helium continuum (Altick & Moore, 1966). The results compared very well with experiment and with the more elaborate close-coupling technique.

An advantage of the configuration interaction method is that the structure of the resonances is more apparent. This feature was exploited in a study of some $^{1,3}D$ resonances in helium (Altick & Moore, 1967), a paper which gave additional physical insight.

The effects of auto-ionization are very large in the alkaline earths so this group was selected for the next investigation. After a generalization of some computer programs to allow Hartree-Fock type radial functions to be calculated, the cross section of beryllium was computed near threshold. (Altick, 1968). This cross section was dominated by auto-ionization, and estimates of its value neglecting this phenomenon would likely be seriously in error. There are still no absolute measurements with which to compare, but some work by Mehlman-Balloffet and Esteva (1969) and more recently Esteva, Mehlman-Balloffet and Romand (1972) show the large features predicted by the theory. No other theoretical calculations are available as of now, but several are underway.

In late 1968 a graduate student, G. N. Bates, took on the task of calculating the magnesium photo-ionization cross section near threshold for a doctoral dissertation. He has recently completed this work, and it has been submitted for publication. His final results agree very well with relative measurements by the workers cited above; again there are large auto-ionization features. There is one absolute measurement at threshold (Ditchburn and Marr 1953), and the experiment differs there from theory by a factor of two. However, there is a strong possibility that the vapor pressure data used by Ditchburn and Marr were in error. Another theoretical calculation (Burges and Seaton, 1960) agrees with Bates' work near threshold.

An important step in generalizing this method so it would be applicable to a larger number of situations would be the development of procedures to properly treat the Coulomb potential as an interaction potential. This potential gives rise to singular matrix elements and one needs to have prescriptions for the treatment of the singularities. This problem was studied while one of us (P. L. Altick) was on a leave of absence during the school year 1967-68, and the mathematics was worked out (Altick, 1969). However, despite an intensive effort stretching over almost two years, the problem

could not be recast in a form suitable for numerical solution and so was finally abandoned. As an offshoot of this project, a simple variational wave function for the ground state of two electron atoms was found (Altick, 1972).

Another graduate student (J. Woodyard) who has received support from this grant is presently pursuing a dissertation problem concerned with rare gas spectra in the vicinity of the first ionization threshold. There are five different Rydberg series in this region, and he is trying to understand why some interact strongly and some do not.

Several other graduate students have not received direct support from this grant, but have successfully completed their degrees in this area (under the guidance of Dr. Altick or Dr. Moore), and have used computer time funded partially from the grant.

Since becoming Chairman of the Physics Department in mid-1969, one of us (E. Neal Moore) has had less time for active research and consequently has received no direct support from the grant. He has remained interested in the work, however, looking at potential astrophysical applications and investigating extrapolation techniques in the complex energy plans as a possible alternative method of computing atomic wave functions.

In summary, the research performed with the help of this grant has produced a method, simpler than close coupling, for the calculation of continuum states of atoms when auto-ionization is present. This method was employed to give the first theoretical cross section for beryllium and magnesium, the results indicating that the values used previously at threshold were sometimes seriously in error. Since threshold values are often used by astrophysicists in abundance estimates, the importance of this work in relation to such estimates is clear.

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